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# On Pairs of Difference Operators
# Satisfying: [D,X] = Id

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## Abstract

Different finite difference replacements for the derivative are analyzed in the context of the Heisenberg commutation relation. The type of the finite difference operator is shown to be tied to whether one can naturally consider $D$ and $X$ to be self-adjoint and skew self-adjoint or whether they have to be viewed as creation and annihilation operators. The first class, generalizing the central difference scheme, is shown to give unitary equivalent representations. For the second case we construct a large class of examples, generalizing previously known difference operator realizations of $[D, X] = Id$.
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## 1. INTRODUCTION

The idea of discrete physics and discrete space–time is a very old one. To the best of our knowledge, the oldest reference in a physical journal is [1][1] and it has been reconsidered many times in the past (see [3] for an extensive bibliographical review on the subject). The basic motivations for all those efforts were: (a) the presence of ultra–violet infinities in the standard quantum field theory; (b) understanding the origin of the fundamental length (mass) scale in the Einstein's general relativity theory.

In recent years there has been a growing number of attempts to find an underlying discrete structure of space–time. At the same time interesting discrete structures have surprisingly emerged within originally continuous models. The most interesting examples can be found in string theory [4], Roger Penrose's spin network calculus [5], the loop representation of quantum gravity [6] (see also [7]), the Bekenstein black hole entropy problem [8, 9, 10, 11, 12] or the recent approach advocated by G. t' Hooft [13,14,15]. Also, it is interesting to mention in this context the old work by Aharonov *et al* [16], where the modular variables for the coordinate and momentum operators have been introduced to describe an infinite slit experiment with magnetic field.

Increasing popularity of discrete models in theoretical physics has been stimulated by several successful attempts to discretize continuous models for technical reasons. This has advanced our understanding of discrete techniques. Here, the best examples are the lattice QCD [17] and the Regge calculus in classical gravity [18].

On the other hand, there have been several attempts to incorporate discrete space–time at the *kinematical* level and to investigate its physical consequences [19, 20]. This line of research can be also associated with the $q$–deformations of the Poincare group [21]. Another interesting approach has been recently proposed by Mazur [22, 12], who has given additional physical arguments in favor of space–time discreteness.

We assume a discrete coordinate space (see also [23]) and investigate its consequences for the Heisenberg commutation relations. This approach is purely kinematical, as the Heisenberg relations are, and does not depend on the details of the underlying dynamics. Such "unusual" realizations of the Heisenberg algebra have also been found in 2D gravity [24]. These representations are not unitarily equivalent to the Schrödinger representation. In particular, they cannot be exponentiated to the Weyl form of the canonical commutation relation.

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[1] The first questions about the world geometry were already posed by Riemann in XIXth century [2].

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To motivate our discussion we first consider the standard quantum mechanical representation of the momentum operator:

$$p_\mu = -i\hbar \frac{\partial}{\partial x^\mu} . \tag{1.1}$$

Hence, the coordinate discretization can be implemented through a derivative discretization:

$$\frac{d}{dx} \longrightarrow D_{\Delta x} , \tag{1.2}$$

where $D_{\Delta x}$ is a discretized derivative (difference) operator and $\Delta x$ is the discretization parameter (usually a fixed coordinate spacing). Even though we will call $D_{\Delta x}$ a discretized derivative it should be noted at this point that initially this is just some difference operator acting, for example, on the space of smooth functions on $\mathbb{R}$. However, such operators can be naturally restricted to act on the space of functions on $\Delta x \times \mathbb{Z}$. It is in this sense that we talk about a discrete derivative.

We will consider a wide class of possible derivative discretization schemes of the form:

$$D_{\Delta x}(M + N + 1) \equiv D_{\Delta x} \equiv \sum_{k=-M}^{+N} \alpha_k \, E_{\Delta x}^k , \tag{1.3}$$

where $\alpha_k$ are real constant coefficients and $M, N$ are integer indices corresponding to the lowest and highest non-zero terms (hence, $\alpha_{-M} \cdot \alpha_N \neq 0$). We take the coefficients $\alpha_k$ to be constant as one would like to have the same definition of the discrete derivative at all points in the coordinate space. The expression will be called $n$–point for $n=M+N+1$. For convenience, let us define the shift operator $E_{\Delta x}^n$ as:

$$E_{\Delta x}^n \, f(x) \equiv E^n \, f(x) = f(x + n \, \Delta x) . \tag{1.4}$$

One can easily check that this operator fulfills the following commutation relations:

$$\begin{aligned}
[E^m, \, E^n] &= 0 , \\
[E^m, \, x] &= m \, \Delta x \, E^m , \\
[E^m, \, x \, E^n] &= m \, \Delta x \, E^{m+n} , \\
[E^m, \, E^n \, x] &= m \, \Delta x \, E^{m+n} .
\end{aligned} \tag{1.5}$$

Several authors have used a purely imaginary $\Delta x$ and $\alpha_k$. This case is not addressed in the present paper and our methods are not directly applicable to it.

In addition, the formal continuum limit reads:

$$\lim_{\Delta x \to 0} E_{\Delta x}^n = 1 . \tag{1.6}$$

In the simplest case: $N = M = 1$ the difference operator can be expressed by the Heine bracket $[\,\cdot\,]_q$ defined for the dimensionless variables $P, q$ as (see Appendix A for its basic properties):

$$H(P, q) \equiv [\,P\,]_q = \frac{(q^P - q^{-P})}{(q - q^{-1})} , \tag{1.7}$$

where $q = e^i$ and $P = -i\frac{\partial}{\partial x}$. This notation is widely used in the context of $q$–deformations and, in particular, to define the $q$–deformed Poincaré group [21] (see also [22]).

This paper is organized as follows. In Sec. 2 we investigate the basic properties of the difference operator (1.3). Sec. 3 is devoted to a construction of the Heisenberg algebra for the operator (1.3) and its conjugate operator $X_{\Delta x}$ when the latter is a bounded operator (finite series). In Sec. 4 we consider the case of unbounded operators. Sec. 5 introduces the momentum formulation of our problem and within this representation we complete our proofs in the unbounded case in Sec. 6. Sec. 7 contains the summary of our results.

## 2. THE DISCRETE DERIVATIVE

In this Section we shall investigate the general properties of the discretized derivative (1.3) and the corresponding momentum operator. We would like to be able to talk about the convergence of discretized operators to the ordinary ones when the parameter $\Delta x$ tends to zero and whenever we can make sense of this limit we will call it *the classical limit*. In particular, we stipulate that for analytic functions:

$$D_{\Delta x} \, f(x) \longrightarrow \frac{d}{dx} f(x) \qquad (\Delta x \to 0) , \tag{2.1}$$

holds pointwise in $x$. Consequently, by writing (2.1) in terms of the translation operator $e^{k\Delta x \frac{d}{dx}}$ we obtain:

$$D_{\Delta x} \, f(x) \equiv \sum_{k=-M}^{+N} \alpha_k \, e^{k\Delta x \frac{d}{dx}} \, f(x) . \tag{2.2}$$

Applying the Taylor expansion to (1.3) at $x = x_i$ we have:

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$$D_{\Delta x}\, f(x_i) \;=\; f(x_i) \sum_{k=-M}^{+N} \alpha_k \;+\; \frac{1}{1!} \frac{df(x_i)}{dx} \sum_{k=-M}^{+N} \alpha_k\, k\, \Delta x \;+$$

$$+\;\ldots\;+\; \frac{1}{n!}\, f^{(n)}(x_i) \sum_{k=-M}^{+N} \alpha_k\, k^n \Delta x^n \;+\;\ldots \tag{2.3}$$

From (2.3), we then get the following two conditions for the coefficients $\alpha_k$ to fulfill (2.1):

$$\sum_{k=-M}^{+N} \alpha_k \;=\; 0\,,$$

$$\sum_{k=-M}^{+N} k\, \alpha_k \;=\; \frac{1}{\Delta x}\,. \tag{2.4}$$

We may also sharpen the notion of a classical limit by specifying the accuracy of the discretization scheme. For example, the coefficients $\alpha_k$ can be chosen to give the best fit to the ordinary derivative by requiring that all terms in (2.3) vanish up to the order $\Delta x^{M+N}$. As a result, in addition to (2.4), the following set of algebraic equations for the coefficients must be satisfied:

$$\sum_{k=-M}^{k=+N} k^n\, \alpha_k \;=\; 0 \qquad \text{for} \quad n = 2, 3, \ldots, (M+N)\,, \tag{2.5}$$

and we get instead of (2.3) the following approximation for the derivative:

$$D_{\Delta x} f(x_i) \;=\; f'(x_i) \;+\; \frac{\Delta x^{M+N+1}}{(M+N+1)!}\, f^{(M+N+1)}(x_i) \times$$

$$\times \sum_{k=-M}^{+M} \alpha_k\, k^{M+N+1} \;+\; o\left(\Delta x^{M+N+1}\right)\,. \tag{2.6}$$

Eqs. (2.4), (2.5) comprise the set of $M+N+1$ linear eqs. for $M+N+1$ coefficients $\alpha_k$ and they can be solved explicitly. The corresponding determinant is the *Vandermonde* determinant and its value is: $\det \|A\| = 1! \cdot 2! \cdot \ldots \cdot (2N)! \neq 0$. Consequently, there exists a unique solution. Its form is given by the following:

**Theorem 1:** *The discrete derivative of the form (1.3) gives the best fit to the ordinary derivative, i.e. it has expansion (2.3) with the first non–vanishing coefficient for $\Delta x^{M+N+1}$, if and only if the coefficients $\alpha_k$ are of the following form:*

$$\alpha_0 \;=\; \frac{-1}{\Delta x} \left[ \sum_{k=1}^{N} \frac{1}{k} \;-\; \sum_{k=1}^{M} \frac{1}{k} \right] ,$$

$$\alpha_k \;=\; \frac{(-1)^{k+1}}{\Delta x} \; \frac{M! \, N!}{k \, (M+k)! \, (N-k)!} \; . \tag{2.7}$$

Higher order terms in the expansion (2.3) cannot vanish, as the system would become overdetermined.

In the symmetric case, i.e. when $M = N$, Theorem 1 implies the symmetry between forward and backward terms. Indeed, in this case the coefficients (2.7) have the following simple properties:

$$\alpha_k(\Delta x) = -\,\alpha_{-k}(\Delta x) = \alpha_{-k}(-\Delta x) \; , \tag{2.8}$$

Moreover, for a fixed $k$,

$$\lim_{N \to \infty} \alpha_k(\Delta x) \;=\; (-1)^{k+1} \, \frac{1}{(\Delta x)k} \qquad (k \neq 0) \; . \tag{2.9}$$

The meaning of (2.9) is explained in Appendix B. Moreover, eq. (2.8) implies the symmetry of the discrete derivative:

$$D_{\Delta x} \;=\; +D_{-\Delta x} \; . \tag{2.10}$$

The operator $D_{\Delta x}$ satisfying (2.10) we shall call **symmetric** (in $\Delta x$). Later on we shall limit ourselves to this case as it preserves the parity symmetry. Discretization schemes and corresponding coefficients satisfying, in addition to (2.4), (2.5) and symmetric we shall call **optimal**. In fact, in the special symmetric case $N = 1$ (2.8) implies that the derivative is optimal and we obtain the well known central difference scheme. The numerical values of the optimal $\alpha$–coefficients for the lowest $(2N+1)$–point schemes are given in the *Table 1* below.

In analogy to (2.2), the optimal derivative can be rewritten as:

$$D_{\Delta x} \, f(x) \;\equiv\; 2 \sum_{k=1}^{N} \alpha_k \, \sinh\left( k\Delta x \frac{d}{dx} \right) \, f(x) \; . \tag{2.11}$$

In particular, for the optimal 3–point (= central difference) discretization scheme we have:

$$D_{\Delta x} \, f(x) \;=\; \frac{1}{\Delta x} \, \sinh\left( \Delta x \frac{d}{dx} \right) \, f(x) \;=\; \frac{1}{i \, \Delta x} \, \sin\left( i \, \Delta x \frac{d}{dx} \right) \, f(x) \; . \tag{2.12}$$

*Table 1. Values of the lowest optimal $\alpha$–coefficients.*

| $N = M$ | $\alpha_1$ | $\alpha_2$ | $\alpha_3$ | $\alpha_4$ | $\alpha_5$ | $\alpha_6$ |
|---------|-----------|-----------|-----------|-----------|-----------|-----------|
| 1 | 1/2 | | | | | |
| 2 | 2/3 | –1/12 | | | | |
| 3 | 3/4 | –3/20 | 1/60 | | | |
| 4 | 4/5 | –1/5 | 4/105 | –1/280 | | |
| 5 | 5/6 | –5/21 | 5/84 | –5/504 | 1/1260 | |
| 6 | 6/7 | –15/56 | 5/63 | –1/56 | 1/385 | –1/5544 |

The representation (2.12) is exactly the derivative represented by the Heine symbol (1.7) ([21, 22]).

Originally, Heisenberg introduced his matrix mechanics by postulating that mathematical operations in classical equations of motion should be reinterpreted (that has led to the correspondence principle). In this spirit Dirac has postulated that the "quantum differentiation" must satisfy the additivity and Leibniz rule. From this he has obtained the fundamental (Heisenberg) commutation relations for coordinates and momenta [25]. We would like to proceed in an analogous way. However, in our case not all general rules for derivatives are satisfied by (1.3), subject to (2.4). The basic properties of the ordinary derivative are listed below along with some comments on how those properties change if one uses $D_{\Delta x}$ instead of $\frac{d}{dx}$:

1. Additivity. Ordinary and discrete derivative are both linear :

$$D_{\Delta x}\ [f(x) + g(x)] = D_{\Delta x}\ f(x) + D_{\Delta x}\ g(x)\ .$$

2. Leibniz rule. The rule for differentiation of the product is not satisfied exactly by (1.3). The deviation is of order $\mathrm{O}\left(\Delta x\right)$ and for the optimal scheme of order $\mathrm{O}\left(\Delta x^{2N}\right)$.

3. Derivative of the composite function. The same result as for the Leibniz rule holds for the derivative of a composite function: $D_{\Delta x}[f \circ g(x)] = D_{\Delta x}f(g(x)) \times D_{\Delta x}g(x) + \mathrm{O}\left(\Delta x^{2N}\right)$.

4. Derivative of monomials. Discrete derivative of the monomial $x^n$ is identical to the ordinary derivative if the discretization scheme is optimal and the exponent $n \leq 2N$. In general, assuming (2.4) and (2.8) we have:

$$D_{\Delta x}(N) \ x^n \ = \ n \ x^{n-1} \ + \ \sum_{k} \sum_{i=2}^{n} \alpha_k \ k^i \ \binom{n}{k} \ \Delta x^i \ x^{n-i} \ . \tag{2.13}$$

5. Heisenberg commutation relation. This will be the subject of the following sections. We shall present a construction of the discrete counterpart of the Schrödinger couple $x$ and $\frac{d}{dx}$ satisfying a discrete analog of the continuous Heisenberg commutation relation: $[\frac{d}{dx}, x] f(x) = f(x)$. Naively, that is, by replacing only $\frac{d}{dx}$ with $D_{\Delta x}$ and using (1.3), we get:

$$[D_{\Delta x}, \ x] \ f(x) \ = \ \Delta x \ \sum_{k} k \ \alpha_k \ f(x + k\Delta x) \ . \tag{2.14}$$

For the optimal discretization we will construct a position operator called $X$ which together with $D_{\Delta x}$ forms a conjugate pair, that is the relation $[D_{\Delta x}, X] = I$ holds on a dense domain in a Hilbert space.

6. Hermicity. In the symmetric case we have a natural Hermitian conjugation induced from the relation $(E_{\Delta x}^n)^\dagger = E_{\Delta x}^{-n}$ The operator $D_{\Delta x}$, like the operator $\frac{d}{dx}$ is formally anti-Hermitian if $M = N$ and $\alpha_k(\Delta x) = -\alpha_{-k}(\Delta x)$ and we have:

$$\int (D_{\Delta x} f(x)) \ g(x) \ dx \ = \ - \int f(x) \ (D_{\Delta x} g(x)) \ dx \ . \tag{2.15}$$

A more detailed analysis will be given in the subsequent sections.


## 3. LIE ALGEBRAIC DISCRETIZATION

The notion of the *Lie algebraic discretization* has been introduced in [26]. It can be described as a special case of representation theory of the enveloping algebra of the Heisenberg algebra in which at least one of the generators is a difference operator. As a result, some linear difference equations have a representation theoretic meaning similar to the D-module interpretation of linear differential equations [27], in particular in Sec. 6. The most important application seems to be to describe quasi-polynomial solutions to a certain class of difference equations. On the other hand the whole procedure has certain appeal of *déjà vue* in the context of basic quantum mechanics and from this point of view one can regard the authors' concept of the Lie algebraic discretization as a quantization procedure.

Following [26], we start with (1.1) and we look for a conjugate operator $X \equiv X_{\Delta x}$ that satisfies:

$$[ D_{\Delta x}, \ X \ ] \ = \ 1 \ , \tag{3.1}$$

with the additional condition ('classical limit'):

$$\lim_{\Delta x \to 0} X_{\Delta x} \ = \ x \ . \tag{3.2}$$

In [26], only the special cases of the forward and backward *Euler schemes* that are not symmetric under reflections (2.10) have been discussed. This can be improved in two ways. Firstly, we can start with the more general discretization scheme (1.3). Secondly, we can require that $D_{\Delta x}$ be formally skew-Hermitian whereas $X_{\Delta x}$ be formally Hermitian relative to some $\star$ anti-involution to ensure a natural physical interpretation.

In [26], it has been shown that for derivatives in the form:

$$D_{\Delta x}^{+} f(x) \equiv \frac{f(x + \Delta x) - f(x)}{\Delta x} \ , \qquad D_{\Delta x}^{-} f(x) \equiv \frac{f(x) - f(x - \Delta x)}{\Delta x} \ , \tag{3.3}$$

we get the Heisenberg algebra for $D^{+}$ and $x(1 - \Delta x D^{-})$:

$$[D^{+}, \ x(1 - \Delta x D^{-})] = 1 \ . \tag{3.4}$$

However, as has been mentioned in Sec. 2, we are not satisfied with the Euler forms of the discrete derivative (3.3), as these schemes are not optimal and symmetric with respect to reflections[2]. In particular, this form of the discrete derivative does not seem to be skew-Hermitian with respect to any natural Hermitian structure. Also, the central difference scheme (and optimal, in general) was shown to enable a consistent formulation of the action principle and the Euler–Lagrange equations in the classical theory [28]. Another possibility would be that the pair $D_{\Delta x}, X$ is a pair of conjugate operators (annihilation and creation operators). But here again, no natural Hermitian structure on the Hilbert space of states seems to induce that.

First, we take up a question of generalizing the results of [26] to a wider class of discrete operators. As the starting point we generalize the form of the coordinate operator used in [26], stipulating the following *Ansatz* :

$$X \ \equiv \ \sum_{k=-N}^{M} \beta_k \, x \, E^k \ , \tag{3.5}$$

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[2] It can be shown that for classical dynamical systems the optimal schemes are closer to continuous derivative with respect to the stability analysis and they preserve the Hamiltonian structure of the phase space, as well [A.Z. Górski and J. Szmigielski, in preparation].

subject to the condition (continuous limit):

$$\sum_{k=-N}^{M} \beta_k \ = \ 1 \ . \tag{3.6}$$

In fact, one can add to (3.5) two additional terms without changing the conclusions. Thus $X$ might be taken to be of the form:

$$X \ \equiv \ \sum_{k=-N}^{M} \beta_k \ x \ E^k \ + \ \sum_{k=-N}^{M} \beta_k' \ E^k \ x \ + \ \sum_{k=-N}^{M} \beta_k'' \ E^k \ . \tag{3.7}$$

The last term commutes with the derivative $D_{\Delta x}$ and does not change commutation relation (3.1). It changes however condition (3.6) replacing it with:

$$\sum_{k=-N}^{M} (\beta_k + \beta_k') = 1 \ , \qquad \sum_{k=-N}^{M} \beta_k'' = 0 \ . \tag{3.8}$$

The second term in the right hand side of (3.7), due to (1.5), has the same commutation relation as (3.5) leading to the substitution:

$$\beta_k \ \longrightarrow \ \beta_k + \beta_k' \ . \tag{3.9}$$

From now on, we restrict our attention to (3.5). From (3.1) we get the following conditions for the $\beta$'s:

$$\sum_{k=-N}^{M} \beta_k \ = \ 1 \ ,$$

$$\Delta x \sum_{\substack{k=-M \\ -N \le n-k \le M}}^{N} \alpha_k \ \beta_{n-k} \ k \ = \ \delta_{n0} \ , \tag{3.10}$$

where $n$ goes from $-(M+N)$ to $+(M+N)$. Here, (3.10) is a set of $(2M+2N+2)$ eqs. for $(2M+2N+2)$ coefficients $\alpha_k, \beta_k$ plus two additional equations (2.4). Hence, the system is formally overdetermined. Let us start with the second equation above (set of $2N+2M+1$ eqs.) and rewrite it as two separate sets, each of size $M+N+1$, corresponding to $n \le 0$ and $0 \le n$ respectively. For simplicity we introduce matrix notation in the $(M+N+1)$–dimensional space of coefficients. Let us define vectors:

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$$\beta = \begin{bmatrix} \beta_{-N} \\ \beta_{-N+1} \\ \vdots \\ \beta_M \end{bmatrix}, \qquad b = \begin{bmatrix} 1/\Delta x \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \qquad (3.11)$$

and two $(N + M + 1) \times (N + M + 1)$ matrices:

$$A_- = \begin{bmatrix} N\alpha_N & \cdots & \cdots & -M\alpha_{-M} \\ (N-1)\alpha_{N-1} & \cdots & -M\alpha_{-M} & 0 \\ \cdots & \cdots & \cdots & \cdots \\ -M\alpha_{-M} & 0 & \cdots & 0 \end{bmatrix},$$

$$A_+ = \begin{bmatrix} N\alpha_N & \cdots & \cdots & -M\alpha_{-M} \\ 0 & N\alpha_N & \cdots & (-M+1)\alpha_{-M+1} \\ \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & 0 & N\alpha_N \end{bmatrix}.$$

$$(3.12)$$

Now, our equations can be rewritten as two sets of equations for the coefficients $\beta_k$ in the following simple form:

$$A_- \, \beta = b, \qquad A_+ \, \beta = b, \qquad (3.13)$$

where the first equations in both sets are identical. The determinants of the systems (3.13) are:

$$\det A_- = (-M \, \alpha_{-M})^{M+N+1}, \qquad \det A_+ = (N^{M+N+1} \, \alpha_N)^{M+N+1}. \qquad (3.14)$$

and (3.13) can be solved explicitly. Indeed, there are three possibilities to consider: 1. both determinants are nonzero (*i.e.* $M \cdot N \neq 0$), 2. one of the determinants is zero, then either $M = 0$ or $N = 0$, 3. both determinants are zero ($M = N = 0$). In the last case the derivative expansion (1.3) consist of one nonzero term ($\alpha_0 E_0$) only and the second condition of (2.4) cannot be fulfilled. In the first case, using Cramer's rule, we get two different solutions to (3.13), hence the system is inconsistent. The only nontrivial possibility is to have the second case. Let us assume that $\alpha_N \neq 0$. Then from the second equation of (3.13) we get the following (unique) solution for $\beta$'s:

$$\beta_{-N} = \frac{1}{N\alpha_N \Delta x}, \qquad \beta_{-N+1} = \ldots = \beta_M = 0, \qquad (3.15)$$

and the first equation of the set (3.10) implies: $\beta_{-N} = 1$ and $\alpha_N = 1/N\Delta x$. Now, consistency of the first eq. of (3.13) implies that the only non–zero $\alpha$'s can be: $\alpha_0$ and

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$\alpha_N$. Finally, eqs. (2.4) are satisfied as well if: $\alpha_0 = -\alpha_N$. Identical solution can be found for $\alpha_{-M} \neq 0$. Hence, we have got the following

**Theorem 2:** *For the discretized derivative operator (1.3) satisfying (2.4) and the coordinate operator in the form (3.5) with condition (3.2) to satisfy Heisenberg commutation relation (3.1) the coefficients $\alpha_k, \beta_k$ must be either in the forward Euler form:*

$$\alpha_k \equiv \alpha_k^F = -\frac{1}{N\,\Delta x}\delta_{k0} + \frac{1}{N\,\Delta x}\delta_{N,k}\ , \qquad \beta_k \equiv \beta_k^F = +\delta_{-N,k}\ , \tag{3.16}$$

*or in the backward Euler form:*

$$\alpha_k \equiv \alpha_k^B = \frac{1}{M\,\Delta x}\delta_{k0} - \frac{1}{M\,\Delta x}\delta_{-M,k}\ , \qquad \beta_k \equiv \beta_k^B = +\delta_{-M,k}\ . \tag{3.17}$$

Thus, for $X$ of the form (3.5) the only way to satisfy (3.1) is to take $D_{\Delta x}$ as the Euler derivatives (3.3). In this case the coordinate operators are:

$$X^{B,F} \ = \ x\,(1 - \Delta x\, D_{N\Delta x}^{\overline{+}}) \ = \ x\, E_{\Delta x}^{\pm N}\ . \tag{3.18}$$

This proves that the Turbiner–Smirnov discretization scheme is unique under conditions (3.1), (3.2), (3.5). Hence, an optimal derivative with the discretized coordinate operator of the form (3.5) cannot satisfy the Heisenberg commutation relation. In fact, this is impossible for any symmetric discretization scheme with finite series in (3.5).

## 4. TRANSCENDENTAL OPERATORS $X$

In the previous Section we have limited our considerations to the coordinate operators (3.5) in the form of a finite series. However, there is still a possibility of having the Heisenberg algebra with the discrete derivative of the form (1.3) and an infinite series for $X$. We shall investigate the algebraic aspects of this problem in this section and a complete, rigorous solution of the problem will be given in Sec. 6. We should mention that the operator $X$ is always unbounded and eventually a special care needs to be exercised when dealing with any expressions involving $X$. In this section we study only formal aspects of our problem leaving aside important questions like the domain of the definition of $X$ or in what sense we understand expressions below involving infinite sums. We will come back to those questions in Sec. 5 and 6.

In the present section we postulate that our coordinate operator has the following form:

$$X = x \sum_{k=-\infty}^{\infty} \beta_m \, E_{\Delta x}^m \, , \tag{4.1}$$

and we have an infinite set of linear algebraic eqs. (3.10) for $n = 0, \pm 1, \pm 2, \pm 3, \dots$ . In addition, the continuous limit condition (3.6) is tentatively taken to mean:

$$\sum_{k=-\infty}^{+\infty} \beta_k = 1 \, . \tag{4.2}$$

Eventually, we will have to regularize this condition since in many examples a direct evaluation of this limit does not make sense.

Defining infinite dimensional matrices and vectors analogous to (3.11), (3.12):

$$\beta_+ = \begin{bmatrix} \beta_{-N} \\ \beta_{-N+1} \\ \beta_{-N+2} \\ \vdots \end{bmatrix} \, , \qquad \beta_- = \begin{bmatrix} \beta_M \\ \beta_{M-1} \\ \beta_{M-2} \\ \vdots \end{bmatrix} \, , \qquad b = \begin{bmatrix} 1/\Delta x \\ 0 \\ 0 \\ \vdots \end{bmatrix} \, , \tag{4.3}$$

$$A_+ = \begin{bmatrix} N\alpha_N & \dots & -M\alpha_{-M} & 0 & \dots & \dots \\ 0 & N\alpha_N & \dots & -M\alpha_{-M} & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{bmatrix} \, ,$$

$$A_- = \begin{bmatrix} -M\alpha_{-M} & \dots & N\alpha_N & 0 & \dots & \dots \\ 0 & -M\alpha_{-M} & \dots & N\alpha_N & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{bmatrix} \, , \tag{4.4}$$

formally, we get, instead of (3.13) the following two sets of eqs.:

$$A_+ \, \beta_+ = b \, , \qquad A_- \, \beta_- = b \, . \tag{4.5}$$

In both sets the first equation is identical and relates at most $(M+N+1)$ coefficients $\beta_m$. Each next equation involves one more (higher order) coefficient that can be explicitly computed. Hence, our system has $(M+N)$ free parameters. In the special case, when $M \cdot N = 0$ the first or last element in each row in (4.4) vanishes and we have $(M+N-1)$ free parameters. This implies for the kernel of operators $A_+, A_-$:

$$D \equiv \dim \ker A_+ = \dim \ker A_- = M + N - \delta_{MN,0} \, . \tag{4.6}$$

Hence, we have proven the following

**Theorem 3:** *For operator $X$ in the form of infinite series (4.1) there is $(M+N-\delta_{MN,0})-$ parameter family of formal solutions to the Heisenberg relation (3.1).*

**Remark:** We do not claim at this point that any of the formal solutions satisfy (4.2).

In the case $M \cdot N \neq 0$ eq. (4.5) imply one algebraic condition for the coefficients $\{\beta_{-N}, \ldots, \beta_M\}$:

$$\sum_{k=-M}^{+N} k \, \alpha_k \, \beta_{-k} \;=\; \frac{1}{\Delta x} \;, \tag{4.7}$$

and the higher coefficients $\beta_k$ ($k > M$ and $k < -N$) can be uniquely determined from:

$$\beta_{M+i} \;=\; \frac{-1}{M\alpha_{-M}} \sum_{k=-M+1}^{+N} k \, \alpha_k \, \beta_{i-k} \;,$$

$$\beta_{-(N+i)} \;=\; \frac{-1}{N\alpha_N} \sum_{k=-M}^{N-1} k \, \alpha_k \, \beta_{-(i+k)} \;, \tag{4.8}$$

where $i = 1, 2, \ldots$ with additional condition (4.2).

In the remainder of this section we shall assume that the coefficients $\alpha_k$ are optimal and the coefficients $\beta_k$ have the symmetry:

$$\beta_k \;=\; \beta_{-k} \;, -N \leq k \leq N \,. \tag{4.9}$$

This implies the symmetry of the discrete coordinate operator with respect to the $\Delta x$ reflections:

$$X_{\Delta x} \;=\; X_{-\Delta x} \;, \tag{4.10}$$

in analogy to the discrete derivative operator (2.10).

Indeed, now we have $N + 1$ $\beta$–parameters $\{\beta_0, \beta_1, \beta_2, \ldots, \beta_N\}$ subject to :

$$\sum_{k=1}^{N} k \, \alpha_k \, \beta_k \;=\; \frac{1}{2\Delta x} \;. \tag{4.11}$$

The higher order coefficients ($\beta_k$ for $|k| > N$) are uniquely determined from:

$$\beta_{N+i} \;=\; \frac{-1}{N\alpha_N} \sum_{k=1}^{N} k \, \alpha_k \, \beta_{i-k} \;-\; \frac{1}{N\alpha_N} \sum_{k=1}^{N-1} k \, \alpha_k \, \beta_{i+k} \;, i = 1, 2, \ldots \;. \tag{4.12}$$

Using induction on $i$ and (4.7) we get the claim:

$$\beta_{-(N+i)} \;=\; \beta_{N+i} \,. \tag{4.13}$$

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We remark that the normalization condition (4.2) can be rewritten as:

$$2 \sum_{k=1}^{+\infty} \beta_k = 1 - \beta_0 , \tag{4.14}$$

*i.e.* we are left with $(N - 1)$ free parameters $\beta$. All considerations in this section were rather formal as we deal with infinite series whose convergence is unclear. In fact, as we shall see below the series might diverge in the usual sense. We discuss in details a concrete example to illustrate this point.

In the case $N = 1$ (4.12) implies the following condition for the $\beta$–coefficients:

$$\beta_{i+2} = \beta_i , \qquad i = 0, 1, 2, \ldots . \tag{4.15}$$

Hence, we have two free parameters: $\beta_0$ and $\beta_1$. The latter can be determined from (4.11), giving:

$$\beta_1 = +1 . \tag{4.16}$$

This provides an exact formula for all odd coefficients in the following compact form:

$$\beta_{2k+1} = (-1)^k , \qquad k = 0, 1, 2, \ldots ,$$
$$\beta_{-(2k+1)} = \beta_{2k+1} , \tag{4.17}$$

and for even coefficients we have:

$$\beta_{2k} = (-1)^k \beta_0 . \tag{4.18}$$

It is clear from (4.17) that our series is indeed divergent and we must redefine the classical limit to make sense of the summation in (4.1). There is no unique way of doing that. We will say more about this in the next section.

At the moment, we are still left with one free parameter, $\beta_0$, and one equation, the normalization condition (4.14). As a special case we can put

$$\beta_0 = 0 . \tag{4.19}$$

Hence, a formal solution for the discretized coordinate operator, $X$, in the $N = 1$ case is (4.1) with $\beta$–coefficients given by:

$$\beta_{2k} = 0 , \qquad \forall k$$
$$\beta_{2k+1} = (-1)^k , \qquad k = 0, 1, 2, \ldots ,$$
$$\beta_{-(2k+1)} = \beta_{2k+1} , \qquad k = 0, 1, 2, \ldots . \tag{4.20}$$

Now, this solution can be compared with the solution found by Frappat and Sciarino [29]. Their solution, after restricting it to 1 dimension, reads:

$$X = x\,\frac{1}{E + E^{-1}} + \frac{1}{E + E^{-1}}x\ . \tag{4.21}$$

There is a formal analogy between their solution and (4.20). To see that analogy one expands the first term in (4.21) at $E = 0$ and the second one at $E^{-1} = 0$. There is, however, an important difference between the approach of the present paper and that of [29]. In their approach, the discretization parameter $\Delta x$ is purely imaginary. As a consequence, the shift operator $E$ is formally Hermitian and positive definite, while the momentum operator corresponding to our $D_{\Delta x}$ is unbounded. Moreover, since the shift is in the imaginary direction it is hard to see what this has to do with a discrete space-time. By contrast, we are treating the shift as a unitary operator, thus retaining the real discretization parameter, which, in turn, ensures that the momentum is bounded.

## 5. MOMENTUM FORMULATION

In this section we reformulate some of the results obtained earlier as well as clarify some of the points left obscure in our discussion of equation (4.21).

The basic idea is to realize the algebra of shift operators as an algebra of multiplication operators on the Hilbert space of square integrable functions on the circle. One can also view this realization as the momentum space counterpart of the content of the preceding sections. Throughout this section $\Delta x = 1$.

At the core of the idea of discretization is that in all operations one proceeds by performing a sequence of discrete steps of size, in this section, 1. This calls for bringing the Fourier transform into the picture. To this end we will first reinterpret (1.5). Our setup is as follows. We consider the unit circle:

$$S^1 = \{z \in \mathbb{C} :\ |z| = 1\} \tag{5.1}$$

and the Hilbert space $H = \mathrm{L}^2(S^1)$. We recall

$$L^2(S^1) = \left\{ f = \sum_{-\infty}^{\infty} a_n z^n :\ \sum_{-\infty}^{\infty} |a_n|^2 < \infty \right\}\ . \tag{5.2}$$

We use the following parametrization of the circle $S^1$: $z = \exp i\theta,\quad \theta \in \mathbb{R} \pmod{2\pi}$. Thus a function $f \in L^2(S^1)$ can be written as:

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$$f(e^{i\theta}) = \sum_{n \in \mathbb{Z}} a_n \, e^{in\theta} \, , \tag{5.3}$$

and $a_n$ are the Fourier coefficients of $f$. Since the shift operator $E$ defined in (1.4) corresponds to the elementary step of unit size we postulate that $E = T_z$, where $T_z$ is the operator of multiplication by $z$. We will say more about multiplication operators towards the end of this section. Till further notice we also suppress writing $T$. Thus we set

$$E^n = z^n \, , \quad x = -z \frac{d}{dz} \, , \quad n \in \mathbb{Z} \, . \tag{5.4}$$

It is routine to check that (1.5) hold. Furthermore we define

$$D(z) := \sum_{k=-M}^{N} \alpha_k \, z^k \, . \tag{5.5}$$

In other words the difference operator becomes now a multiplication by a Laurent polynomial in $z$. We might observe that the operator $x$ above is one of the generators of the Virasoro algebra (with the trivial central term), called, $L_0$. Now we reinterpret equations (2.4) and (2.5). We see that (2.4) goes into

$$D(z = 1) = 0 \, , \quad (L_0 D)(z = 1) = -1 \, . \tag{5.6}$$

Similarly, (2.5) goes into

$$(L_0^n D)(z = 1) = 0 \, , \quad \text{for} \quad n = 2, 3, \dots, (M + N) \, . \tag{5.7}$$

Now, it is immediate that the coordinate operator $X$ should be sought (see (3.4)) in the form

$$X = -z \sum_{n=-\infty}^{\infty} \beta_n \, \frac{d}{dz} z^n \, , \tag{5.8}$$

where

$$\sum_{n=-\infty}^{\infty} \beta_n = 1 \, . \tag{5.9}$$

Let us now, at least formally, introduce the function $h(z) = \sum_{-\infty}^{\infty} \beta_n z^n$. From the above condition we get that $h(1) = 1$. Moreover $X$ can be written

$$X(z) = L_0 h(z) = -zh(z)\frac{d}{dz} - zh'(z) \ . \tag{5.10}$$

As was already explained earlier, we can in fact ignore the second part and look for $X$ in the form:

$$X(z) = -f(z)\frac{d}{dz} \ , \qquad f(1) = 1 \ . \tag{5.11}$$

Thus $X$ is formally an element of the Virasoro algebra. We want that

$$[D(z), X(z)] = \left[ f(z)\frac{d}{dz}, D(z) \right] = 1 \ , \tag{5.12}$$

where $D(z)$ is a function (Laurent polynomial) defined previously. We therefore obtain that:

$$f(z) \ D'(z) = 1 \ , \tag{5.13}$$

which formally implies

$$f(z) = \frac{1}{D'(z)} \ . \tag{5.14}$$

We note that the condition $f(1) = 1$ is automatically satisfied as a consequence of the second condition imposed on $D$. However, it is important to underscore the fact that the latter expression can only be understood formally at this stage of our analysis. Yet, there are some special cases when we do not expect to have any difficulties. For example, if $D(z) = A + Bz$, that is $M = 0$, $N = 1$. Then we impose the following conditions:

$$D(1) = 0 \ , \quad D'(1) = 1 \ , \tag{5.15}$$

which gives $D(z) = z - 1$ and, consequently, $f(z) = 1$. Thus we get the pair $D(z) = z - 1$, $X(z) = -\frac{d}{dz}$ which clearly satisfies (5.12). Using (5.10) we get that in this case $h(z) = \frac{1}{z}$. Hence $\beta_{-1} = 1$ and $\beta_i = 0, i \neq -1$. Going back to the difference operator realization we get that $D = E - I$, $X = xE^{-1}$ which is the pair found in [26] for $\Delta x = 1$. We can contrast this example with that of the symmetric discretization scheme for which $D(z) = \frac{1}{2}(z - z^{-1})$. In that case $f(z) = \frac{2z^2}{1+z^2}$ which is not bounded on the unit circle and consequently $f(z)$ is not a multiplier (that is the multiplication by $f$ is not a bounded operator on $L^2(S^1)$). This example is explained in detail in the next section.

However, there are many cases for which $f$ is a multiplication operator on the circle. We present now a general construction of $X$ for which $f$ is a multiplier. One can view this construction as a generalization of [26].

First, we review a few elementary facts from the theory of doubly infinite Toeplitz operators. Initially, we can consider a vector space of sequences $a = \{a_n\}_{n \in \mathbb{Z}}$ such that $\sum_{n \in \mathbb{Z}} |a_n|^2 < \infty$. This space, called $\ell^2$, is isomorphic to $L^2(S^1)$, the fact well known from the theory of Fourier series. On $\ell^2$ we introduce a linear operator $T_c$:

$$a_m \to \sum_{n \in \mathbb{Z}} c_{m-n} a_n \ , \tag{5.16}$$

where $c = \{c_n\}_{n \in \mathbb{Z}}$ is a sequence of numbers. It is known, that $T_c$ is a bounded operator on $\ell^2$ iff $c$ is a sequence of the Fourier coefficients of an essentially bounded function on $S^1$. We recall that $\phi(\theta)$ is an essentially bounded function on $S^1$ if it is bounded almost everywhere there. The isomorphism between $\ell^2$ and $L^2$ allows one to study the Toeplitz operator $T_c$ as acting on $L^2(S^1)$. We will say that $\phi(\theta)$ is a symbol of $T_c$ if under this isomorphism $T_c$ acts on $L^2(S^1)$ as:

$$(T_c f)(\theta) = \phi(\theta) f(\theta) \ , \qquad f \in L^2(S^1) \ . \tag{5.17}$$

Because of this relation we often write $T_\phi$ to denote the Toeplitz operator with symbol $\phi$. We will need in this section one more result from the theory of Toeplitz operators. The result below gives a complete description, in terms of symbols, of invertible Toeplitz operators.

**Lemma 1:** $T_\phi$ is invertible if and only if $1/\phi$ is essentially bounded. If this holds, $T_\phi^{-1} = T_{1/\phi}$.

Now we apply this lemma to our problem. Let us first consider a Laurent polynomial $g(z)$ such that $Res_{z=0} g = 0$ and $g$ is nowhere zero on $S^1$. We can normalize such a $g$ to satisfy $g(1) = 1$. Now we define

$$D(e^{i\theta}) := i \int_0^\theta e^{it} g(e^{it}) \ dt \ , \tag{5.18}$$

where we used $dz = ie^{i\theta} d\theta$. Observe that since there is no $z^{-1}$ in $g$, $D(z)$ is again a Laurent polynomial satisfying (5.6). Now we set $f(z) = \frac{1}{g(z)}$. We see that $f(z)$ is bounded on $S^1$ so, by the lemma above, $T_f$ is then the bounded inverse of $T_g$. Now we define the operator $X(z) = -T_f \frac{\partial}{\partial z}$: $C^\infty(S^1) \to C^\infty(S^1)$. By exactly the same computation as the one leading up to (5.5) we obtain that on $C^\infty \subset L^2(S^1)$, $X(z)$ and $D(z)$ so defined satisfy the Heisenberg commutation relation as well as (5.6).

Our original setup has been formulated in terms of the $\ell^2$ space. Now we would like to return to it. The map which maps back $L^2(S^1)$ to $\ell^2$ is given by the Fourier series method: $f \to \{\hat{f}(n)\}_{n \in \mathbb{Z}}$, where $\hat{f}(n)$ is the $n$-th Fourier coefficient of $f$. We recall that using (5.10) we can describe the coefficients $\beta_n$ as:

$$\beta_n = \hat{f}(n+1), \quad n \in \mathbb{Z} . \tag{5.19}$$

**Example**: $g(z) = a + bz^{-2}, |a/b| \neq 1$. The condition $g(1) = 1$ gives $a + b = 1$. Thus $D(z) = az + (1 - 2a) + (a - 1)z^{-1}, |a/(1 - a)| \neq 1$. We have two cases to consider depending on whether $|a/(1 - a)| < 1$ (Case 1) or $|a/(1 - a)| > 1$ (Case 2).

*Case 1:* $f(z) = z^2 \frac{1}{az^2 + (1-a)}$.

We observe that $f$ is analytic inside the unit circle $S^1$ and thus its Fourier expansion coincides with its Taylor expansion around $z = 0$. We get

$$\hat{f}(n) = \begin{cases} \frac{(-1)^{(n-2)/2}}{1-a}(\frac{a}{1-a})^{(n-2)/2}, & \text{if } n \geq 2 \text{ and } n \text{ is even;} \\ 0, & \text{otherwise.} \end{cases} \tag{5.20}$$

Thus

$$\beta_n = \begin{cases} \frac{(-1)^{(n-1)/2}}{1-a}(\frac{a}{1-a})^{(n-1)/2}, & \text{if } n \geq 1 \text{ and } n \text{ is odd;} \\ 0, & \text{otherwise.} \end{cases} \tag{5.21}$$

*Case 2:* $f(z) = \frac{1}{a+(1-a)z^{-2}}, |a/(1 - a)| > 1$.

We observe that $f$ is analytic outside of the unit circle $S^1$ and thus its Fourier expansion coincides with its Taylor expansion around $z = \infty$. We get:

$$\hat{f}(n) = \begin{cases} \frac{(-1)^{n/2}}{a}(\frac{1-a}{a})^{(-n)/2}, & \text{if } n \leq 0 \text{ and } n \text{ is even;} \\ 0, & \text{otherwise.} \end{cases} \tag{5.22}$$

Consequently,

$$\beta_n = \begin{cases} \frac{(-1)^{(n+1)/2}}{a}(\frac{1-a}{a})^{(-n-1)/2}, & \text{if } n \leq -1 \text{ and } n \text{ is odd;} \\ 0, & \text{otherwise.} \end{cases} \tag{5.23}$$

This example illustrates very well the fact that the optimal discretization is special even from the point of view of the Heisenberg commutation relations. Indeed the case excluded from the example is $a = 1/2$ which is precisely the optimal case. We can get, however, some information about this case making $a$ approach $1/2$. This allows us to discuss the formal solution (4.20). One way of interpreting this solution relies on a regularization of $D$ which essentially amounts to moving the zeros of $D'$ off the unit circle. We now present a simple example of such a regularization. First we set $a = \frac{1}{2} - \epsilon, \epsilon > 0$. We

observe that $|\frac{a}{(1-a)}| < 1$, so, we are dealing with the first case above. Directly from (5.21) we get:

$$\beta_n(\epsilon) = \begin{cases} \frac{(-1)^{(n-1)/2}}{1/2-\epsilon}(\frac{1/2-\epsilon}{1/2+\epsilon})^{(n-1)/2}, & \text{if } n \geq 1 \text{ and } n \text{ is odd;} \\ 0, & \text{otherwise.} \end{cases} \quad (5.24)$$

It is interesting to note that

$$\beta_n(0) = \begin{cases} 2(-1)^{(n-1)/2}, & \text{if } n \geq 1 \text{ and } n \text{ is odd;} \\ 0, & \text{otherwise.} \end{cases} \quad (5.25)$$

This is a formal solution to (4.7) and (4.8), with no symmetry condition imposed on $\beta$'s. It has exactly the same status as the symmetric solution (4.20). Thus we see that the formal solutions of Section 5 can be justified through an appropriate regularization. In addition we have to properly interpret (4.2) (classical limit). It makes sense to consider this expression for $\epsilon \neq 0$. Then, as it is easy to check,

$$\sum_{k=-\infty}^{\infty} \beta_k(\epsilon) = 1. \quad (5.26)$$

The same expression does not make sense for $\epsilon = 0$, clearly indicating that one cannot interchange $\lim_{\epsilon \to 0}$ with $\sum$.

The final item we would like to discuss in this section is the question of Hermicity or rather lack thereof. In our formulation the pair $D$ and $X$ may not necessarily consist of (even formally) Hermitian or adjoint elements. This is plain, for example, if one looks at the pair $D = E - 1$ and $X = xE^{-1}$ or even more general pairs found above. One could, however, make this pair adjoint to each other, thus turning $D$ and $X$ into a pair consisting of a creation and annihilation operators, by constructing a proper representation space. One possibility would be to consider a Fock representation, which carry an, essentially, unique Hermitian form. Thus, for the last example, the completion of the space $span\{e_n = X^n 1, n \geq 0\}$ with respect to the inner product $< e_m, e_n >= \delta_{m,n}n!$ gives us a Fock space on which $D$ acts as an annihilation operator and $X$ acts as a creation operator respectively, and both act as difference operators. Another possibility is to consider a coherent representation, i.e. such which is generated from the vector $v : Dv = \lambda v, \lambda \in \mathbb{C}$, whose special case is the Fock representation obtained for $\lambda = 0$. In the case of $D = E - 1$ the vacuum state $v$ is a quasiperiodic function satisfying $v(x+1) = (\lambda+1)v(x)$. One obtains the representation space as the $span\{e_n = X^n v, n \geq 0\}$ and the unique Hermitian form is defined by $< v, v >= 1, < e_m, e_n >=< v, D^m X^n v >$ where in the last expression one moves $X$ to the left and $D$ to the right making use of (5.12), the formula $< u, X^n w >=< D^n u, w >$ and $Dv = \lambda v$.

In the next section we study the optimal discretization for which we show that one can construct pairs of Hermitian (self-adjoint) operators $D$ and $X$.

## 6. MOMENTUM FORMULATION APPROACH TO OPTIMAL DISCRETIZATION

Now we take on the case of the optimal discretization. Thus $M = N$ throughout this section. Also, in this section we are interested in self-adjoint pairs $X, P$ relative to the standard inner product on $L^2(S^1)$. For convenience we multiply $D$ from previous sections by $1/i$ and denote the resulting function by $D_N$.

The problem of classifying the pairs of operators satisfying Heisenberg commutation relations under an additional assumption that one of the operators be bounded was considered in [30]. Since our difference operators are bounded, we are studying a special case of that classification, included in [30], in particular in Theorem 8.5 therein. The approach below is direct, however, and can be used as an introduction to a more encompassing treatment of [30]. Moreover, we have a different physical motivation, our interest lies in concrete bounded operators explicitly given by difference operators, reflecting the underlying assumption that the coordinate space is discrete. We recall some basic definitions from [30]. Let $H$ denote a separable Hilbert space over $\mathbb{C}$.

**Definition:** *Let $P$, $Q$ be operators in $H$, and $\Omega$ a dense subspace of $H$. We call $(P, Q)$ a conjugate pair on $\Omega$ iff*

*(K1) $P$ and $Q$ are symmetric, $\Omega \subset D(P) \cap D(Q)$,*

*(K2) $P\Omega \subset \Omega$, $Q\Omega \subset \Omega$,*

*(K3) $P = \overline{P/\Omega}$, $Q = \overline{Q/\Omega}$,*

*(K4) $Q$ is bounded.*

In this section we essentially show that our $X$ and $D_N$ form a conjugate pair in the above sense.

We start with

**Lemma 2:** *Let $D_N(z)$ be optimal, then $D'_N(z)$ has two simple roots on the circle $S^1$.*

**Proof:** Since $z = e^{i\theta}$, $0 \leq \theta < 2\pi$, we want to show that $\frac{d}{d\theta}D_N \equiv D'_N(\theta)$ has exactly two zeros for $\theta \in [0, 2\pi)$.

To derive $D'_N(\theta)$ we first compute $D_N(\theta)$. We get that

$$D_N(\theta) \;=\; 2 \sum_{k=1}^{N} \frac{(-1)^{k+1}}{k} \frac{(N!)^2}{(N+k)!(N-k)!} \, \sin k\theta \; .$$

Hence,

$$D'_N(\theta) \;=\; 2 \sum_{k=1}^{N} (-1)^{k+1} \frac{(N!)^2}{(N+k)!(N-k)!} \, \cos k\theta$$

or, in terms of $z$:

$$D'_N(\theta) = \sum_{\substack{k=-N \\ k\neq 0}}^{N} \frac{(-1)^{k+1}(N!)^2}{(N+k)!(N-k)!} \, z^k =$$

$$= \frac{(-1)^{N+1}(N!)^2}{(2N)!} \, z^{-N} \sum_{\substack{k=-N \\ k\neq 0}}^{N} (-1)^k \binom{2N}{N} z^k =$$

$$= \frac{(-1)^{N+1}(N!)^2}{(2N)!} \, z^{-N} \left[ (1-z)^{2N} - (-1)^N \binom{2N}{N} z^N \right] \; .$$

Thus it suffices to show that the polynomial $(1-z)^{2N} - (-1)^N \binom{2N}{N} z^N$ has exactly two

zeros for $z \in S^1$. Indeed, we obtain: $\left[ \frac{(1-z)^2}{z} \right]^N = (-1)^N \binom{2N}{N}$ or $\sin^2 \frac{\theta}{2} = \frac{1}{4} \sqrt[N]{\binom{2N}{N}}$.

This equation has two solutions, provided: $\frac{1}{4} \sqrt[N]{\binom{2N}{N}} < 1, \quad N \geq 1.$

Indeed, for $N=1$ we get $\frac{1}{4}\cdot 2 < 1$ and there are two roots, $\theta = \frac{\pi}{2}, \frac{3}{2}\pi$. Now, we proceed
by induction. First we observe that the above inequality is equivalent to: $\binom{2N}{N} < 4^N$.
We already proved it for $N=1$. We note that:

$$\binom{2N+2}{N+1} = \binom{2N}{N} \frac{(2N+1)(2N+2)}{(N+1)^2} = \binom{2N}{N} \frac{2(2N+1)}{(N+1)} \; ,$$

and we use the induction hypothesis to prove the claim.

To prove that the zeros are simple we show that $\frac{d}{dz}[(1-z)^{2N} - (-1)^N \binom{2N}{N} z^N]$ is

not zero there. Using that $(1-z)^{2N} - (-1)^N \binom{2N}{N} z^N = 0$ we obtain that this derivative
can be zero if and only if $2z^2 - 2z - 1 = 0$. Since this equation has two real zeros not equal
to $\pm 1$ we conclude that the zeros of $D'_N(\theta)$ are simple. $\blacksquare$

Now, we turn to the problem of the localization of those zeros. We will show that
both zeros move towards $\theta = \pi$ as $N \to \infty$. First we prove three technical lemmas.

**Lemma 3:**

$$\frac{(1+\frac{1}{2N})}{(1+\frac{1}{N})} < \frac{1+\frac{1}{2(N+1)}}{1+\frac{1}{N+1}} \ , \qquad N \geq 1 \ .$$

**Proof:** Consider $(1+\frac{1}{2N})(1+\frac{1}{N+1}) = \frac{2N^2+5N+2}{2N(N+1)}$ and $(1+\frac{1}{N})(1+\frac{1}{2(N+1)}) = \frac{2N^2+5N+3}{2N(N+1)}$. Hence, $(1+\frac{1}{2N})(1+\frac{1}{N+1}) < (1+\frac{1}{N})(1+\frac{1}{2(N+1)})$ which implies the claim. ∎

The next lemma improves on the estimate used in the course of the proof of Lemma 2.

**Lemma 4:**

$$\binom{2N}{N} < 4^N \left[\frac{(1+\frac{1}{2N})}{(1+\frac{1}{N})}\right]^N \ , \qquad N \geq 1 \ .$$

**Proof:** The proof goes by induction on $N$. The only nontrivial step is to observe that:
$\binom{2(N+1)}{N+1} = \binom{2N}{N} \frac{4(1+\frac{1}{2N})}{(1+\frac{1}{N})}$ which, by the induction hypotheses, implies:
$\binom{2(N+1)}{N+1} < 4^{N+1} \left[\frac{(1+\frac{1}{2N})}{(1+\frac{1}{N})}\right]^{N+1}$.
Now, the claim follows from Lemma 3. ∎

Finally, we have:

**Lemma 5:** *The sequence* $a_N = \frac{1}{4} \sqrt[N]{\binom{2N}{N}}$ , $N = 1, 2, \dots$ *is increasing and*

$\lim_{N\to\infty} a_N = 1$.

**Proof:** By Lemma 4, $a_N < \frac{1+\frac{1}{2N}}{1+\frac{1}{N}}$. Hence,

$$4\binom{2N}{N} a_N < 4\binom{2N}{N} \frac{(1+\frac{1}{2N})}{(1+\frac{1}{N})} \ .$$

The left hand side equals $\binom{2N}{N}^{\frac{N+1}{N}}$ , from which we get $\binom{2N}{N}^{\frac{N+1}{N}} < \binom{2(N+1)}{(N+1)}$,
which implies that: $a_N < a_{N+1}$. To compute $\lim_{N\to\infty} a_N$ we observe that
$\lim_{N\to\infty} \exp\frac{1}{N}[\ln(2N)! - 2\ln(N)!]$ can be computed using the Stirling formula:

$$\Gamma(x) = e^{-x} x^{x-\frac{1}{2}} (2\pi)^{1/2} \left[1 + \frac{1}{12x} + \cdots\right] \ ,$$

valid for large $x$. Thus

$$\lim_{N\to\infty} a_N = \frac{1}{4} \lim_{N\to\infty} \exp\frac{1}{N}\left[\ln(2N+1)^{2N+\frac{1}{2}} - 2\ln(N+1)^{N+\frac{1}{2}}\right] =$$
$$= \frac{1}{4} \lim_{N\to\infty} e^{2\ln\left(\frac{2N+1}{N+1}\right)} = 1 \ ,$$

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thus completing the proof. ∎

To find the roots of $D'_N(\theta)$ we solve $\sin^2 \frac{\theta_N}{2} = a_N$. By Lemma 5 we see that $\theta_N$'s are approaching $\pi$ as $N$ increases. Table 2 illustrates this phenomenon numerically.

*Table 2. Roots of $D'_N$.*

| N | 1 | 10 | 100 | 2 500 | 10 000 |
|---|---|----|-----|-------|--------|
| root 1 | $\frac{1}{2}\pi$ | 2.32 | 2.80 | 3.06 | 3.10 |
| root 2 | $\frac{3}{2}\pi$ | 3.96 | 3.48 | 3.27 | 3.19 |

Let us denote by $\theta_N^+$, $\theta_N^-$ the zeros of $D'_N(\theta)$, $\theta_N^\pm \in [0, 2\pi]$. Then on the intervals $I_N^1 = (\theta_N^- - 2\pi, \theta_N^+)$, $I_N^2 = (\theta_N^+, \theta_N^-)$, $D_N(\theta)$ is monotone and thus $D_N(\theta)$ has an inverse which we denote by $\phi_N^1$ and $\phi_N^2$ respectively. Now, we observe that the Hilbert space $H = L^2(S^1) \simeq L^2([\theta_N^- - 2\pi, \theta_N^-])$ admits the direct sum decomposition: $H = L^2(I_N^1) \oplus L^2(I_N^2)$. Moreover, we have:

$$L^2(I_N^i) \simeq L^2(D_N(I_N^i)) , \quad \tau_i : \ \psi(\theta) \to |(D'_N \circ \phi_N^i)(y)|^{-1/2} \ \psi(\phi_N^i(y)) ,$$

where $y = D_N(\theta)$ and $i = 1, 2$. Now we show that $\tau$ is a unitary isomorphism.

**Lemma 6:** $\tau_i$ *is a unitary isomorphism, $i = 1, 2$.*

**Proof:**

$$\langle \psi_1 | \psi_2 \rangle = \int_{I_N^i} \overline{\psi_1(\theta)} \psi_2(\theta) \ d\theta = \int_{D_N(I_N^i)} \overline{\psi_1(\phi_N^i(y))} \psi_2(\phi_N^i(y)) \left| \frac{dy}{d\theta} \right|^{-1} dy .$$

Observe, however, that $\left| \frac{dy}{d\theta} \right| = |(D'_N \circ \phi_N^i)(y)|$. Hence,

$$\langle \psi_1 | \psi_2 \rangle_{L^2(I_N^i)} = \int_{D_N(I_N^i)} \overline{(\tau_i \psi_1)}(y) \ (\tau_i \psi_2)(y) \ dy = \langle \tau_i \psi_1 | \tau_i \psi_2 \rangle_{L^2(D_N(I_N^i))} ,$$

that ends the proof. ∎

We will need an explicit form of the inverse of $\tau_i$. A simple computation yields:

$$\tau_i^{-1} : \ \phi \to |D'_N(\theta)|^{1/2} \phi(D_N(\theta)) , \quad \theta \in I_N^i , \quad \phi \in L^2(D_N(I_N^i)) .$$

Now, we want to define the skew-Hermitian part of the operator $\frac{1}{D_N'(\theta)}\frac{d}{d\theta}\frac{1}{D_N'(\theta)}$ on $L^2(D_N)$. It is easier, however, to consider first its push-forward under $\tau$:

$$\frac{1}{2}\tau_i \circ \left[\frac{1}{D_N'(\theta)}\frac{d}{d\theta} + \frac{d}{d\theta}\frac{1}{D_N'(\theta)}\right] \circ \tau_i^{-1}\phi(y) =$$

$$= \frac{1}{2}\tau_i \circ \left[\frac{1}{D_N'(\theta)}\frac{d}{d\theta} + \frac{d}{d\theta}\frac{1}{D_N'(\theta)}\right](\mathrm{sign}(D_N'(\theta))\,D_N'(\theta))^{1/2}\,\phi(D_N(\theta)) =$$

$$= \frac{1}{2}\tau_i \circ \left[\frac{1}{D_N'(\theta)}\,\phi(D_N(\theta)) + 2\frac{\mathrm{sign}D_N'(\theta)}{(\mathrm{sign}(D_N'(\theta))D_N'(\theta))^{1/2}}\,\partial_\theta\phi(D_N(\theta))\right] =$$

$$= \tau_i \circ \frac{\mathrm{sign}D_N'(\theta)}{(\mathrm{sign}(D_N'(\theta))D_N'(\theta))^{1/2}}\,\partial_\theta\phi(D_N(\theta)) =$$

$$= |D_N' \circ \varphi_N^i(y)|^{-1/2}\,\frac{\mathrm{sign}(D_N'(\theta))\circ\varphi_N^i)(y)}{|D_N'(\theta)\circ\varphi_N^i(y)|^{1/2}}\,\frac{\partial}{\partial\varphi_N^i(y)}\phi(y) =$$

$$= \frac{1}{D_N'\circ\varphi_N^i)(y)}\,\frac{\partial}{\partial\varphi_N^i(y)}\phi(y)\ .$$

Since $\frac{\partial}{\partial y} = \frac{\partial\varphi_N^i(y)}{\partial y}\frac{\partial}{\partial\varphi_N^i(y)}$ we need to compute $\frac{\partial\varphi_N^i(y)}{\partial y}$. To this end we simply observe that $(\varphi_N^i \circ D_N)(\theta) = \theta$. Hence,

$$\frac{d\varphi_N^i}{dy} = \frac{1}{D_N'(\theta)} = \frac{1}{(D_N' \circ \varphi_N^i)(y)}\ .$$

This implies:

$$\left(\tau_1 \circ \frac{1}{2}\left[\frac{1}{D_N'(\theta)}\frac{d}{d\theta} + \frac{d}{d\theta}\frac{1}{D_N'(\theta)}\right] \circ \tau_1^{-1}\right)(y) = \frac{\partial}{\partial y}\ ,\quad y \in D_N(I_N^i)\ .$$

We thus have the following important

**Theorem 4:** *Let $X_N = \frac{i}{2}\left[\frac{1}{D_N'(\theta)}\frac{d}{d\theta} + \frac{d}{d\theta}\frac{1}{D_N'(\theta)}\right]$ be defined on a dense set $S \in L^2(S^1)$. Then $X$ is unitary equivalent to $i\frac{\partial}{\partial y}\Big|_{L^2(D_N(I_N^1))} \oplus i\frac{\partial}{\partial y}\Big|_{L^2(D_N(I_N^2))}$, defined on the dense space $\tau_1(S \cap L^2(I_N^1)) + \tau_2(S \cap L^2(I_N^2))$.*

We can prove a similar statement for $D_N(\theta)$. We have: $\tau_i \circ D_N(\theta) \circ \tau_i^{-1}\phi(y) = \tau_1 \circ D_N(\theta)|D_N'(\theta)|^{1/2}\phi(D_N(\theta)) = |D_N' \circ \varphi^i(y)|^{-1/2}D_N \circ \varphi^i(y)|D_N' \circ \varphi^i(y)|^{1/2}\phi(D_N \circ \varphi^i)(y)$ $= y\phi(y)\ ,\ \ y \in D_N(I_N^i)$. Hence

**Theorem 5:** *Let $P_N$ be the operator of multiplication by the function $D_N$. Then $P_N$ is unitary equivalent to $y\Big|_{L^2(D_N(I_N^1))} \oplus y\Big|_{L^2(D_N(I_N^2))}$.*

**Corollary:** The pair $Q = D_N$ and $P = -X$ is a conjugate pair on $\Omega$, where: $\Omega = \tau^{-1}(S_1) \oplus \tau^{-1}(S_2)$, $S_i = \{f \in L^2(D_N(I_N^i)), f$ is absolutely continuous, $f = 0$ on the boundary of $D_N\}$, $i = 1, 2$.

**Remark** Observe that $X$ is closed and symmetric on $\Omega$. We discuss its self-adjoin extensions below.

First, however, we determine the spectrum of $D_N$ or to be more precise $T_{D_N}$. By the well known theorem on Toeplitz operators [31]: $\text{Spec}(T_{D_N})$ = essential range of $D_N$ = range of $D_N$, where the latter is a consequence of continuity. Because $X_N$ decomposes into a direct sum of operators of the type $i\frac{d}{dy}$ on the finite intervals $D_N(I_N^i)$ we present a brief description of basic features of such operators. For convenience we take a finite interval $[-1, 1]$. The following discussion is based on [32] and all the details can be found there. The operator $i\frac{d}{dy}$ is known to have a one parameter family of self–adjoint extensions. More precisely, let us set $i\frac{d}{dy} = T_\alpha$, defined on $D(T_\alpha) = \{\varphi : \varphi$ is absolutely continuous and $\varphi(-1) = \alpha\varphi(1)\}$, where $\alpha \in \mathbb{C}$, $|\alpha| = 1$.

To interpret $\alpha$ we solve the eigenvalue problem: $i\frac{d}{dy}\psi = \lambda\psi$ with $\psi(-1) = \alpha\psi(1) = e^{i\varphi_0}\psi(1)$, $\alpha = e^{i\varphi_0}$, $\varphi_0 \in [0, 2\pi)$. Thus we get: $\psi(y) = e^{i\lambda y}$ and $e^{-i\lambda} = e^{i\varphi_0}e^{i\lambda}$ from which it follows that $2\lambda + \varphi_0 = 2\pi n$, $n \in \mathbb{Z}$. Hence, $\lambda = \lambda_n = n\pi - \frac{\varphi_0}{2}$, $n \in \mathbb{Z}$. The appearance of $\pi$ is accidental and can easily be removed by rescaling of $T_\alpha$. The spectrum of $T_\alpha$ is a lattice of physical positions. We would like to point out that there is no canonical way of identifying this lattice with the lattice we have started with. It seems to be compelling in fact to consider as a real physical space the lattice of eigenvalues of $T_\alpha$ and the corresponding Hilbert space $L^2(D_N(I_N^1))$, for example. Thus we would, so to speak, avoid the "spectrum doubling " problem by decree. On the other hand this would have to be interpreted quantum mechanically as saying that the process of quantization amounts in this case to finding an irreducible representation of the Heisenberg commutation relations with the additional condition that the spectrum of would be position is discrete. This representation would then have a relation to the calculus of difference operators as described above, yet, the physical Hilbert space would be only "half" of the Hilbert space that naturally carries the action of difference operators.

To close this section we would like to mention that the optimal discretization has a very nice property that $\lim_{N\to\infty} D_N(\theta) = \theta$. This fact is proven in Appendix B. It is only in this case that we get an irreducible representation of the Heisenberg commutation relations in the case of the optimal discretization.


## 7. SUMMARY AND CONCLUSIONS

In this paper we have investigated a wide class of discretization schemes for the derivative and/or momentum operator defined by (1.3). The optimal subclass of these schemes

has been distinguished, that give the best fit to the continuous operators and are symmetric with respect to the space reflections. The particular form of those schemes has been determined in Sec. 2. It has been shown that the solution found in [26] is the only solution in the form of finite series for the operator $X$. We also have determined that the commutation relation for the annihilation–creation type of operators can be satisfied for a large class of difference operators, thus extending the result of [26], if one admits $X$ in a form of an infinite series in $E$.

Our analysis in Sec. 6 has shown that upon quantization the classically different optimal discretization schemes are all unitary equivalent. As a result, the number of points used to "delocalize" $\frac{d}{dx}$ is unessential. For a fixed number of these points, say $2N + 1$, the representation of the canonical commutation relations is reducible. Furthermore, by the result of Appendix B its irreducible components are unitary equivalent to the case with an infinite $(N \to \infty)$ number of points.

Further extensions of this work can be done in several directions. First, one can investigate the case of an imaginary shift, as has been mentioned in Sec. 1. Second, more general Ansatz for the $P$ and $X$ operators can be analyzed. In particular, we suggest that the representation used in [24] can be included into our scheme by considering operator $X$ being a nonlinear function of $x$. Finally, it would be interesting to study simple quantum mechanical systems within our approach.

## A p p e n d i c e s

## Appendix A: Heine symbols

The Heine symbol defined by (1.7) have pretty interesting behavior. The deformation

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parameter $q \geq 0$ is usually bound to the (complex) region: $|q| \leq 1$ and it is parameterized exponentially by a (dimensionless) physical parameter $l$:

$$q = \exp\left(\frac{il}{2}\right) . \qquad (A.1)$$

The above parametrization allows us to rewrite the Heine symbol (1.7) in the following widely used form:

$$[P]_q \equiv \frac{\sin(\frac{lP}{2})}{\sin(\frac{l}{2})} = \frac{\sinh(\frac{ilP}{2})}{\sinh(\frac{il}{2})} , \qquad (A.2)$$

Function $H(P, q)$ is antisymmetric in $P$:

$$H(P, q) = -H(-P, q) . \qquad (A.3)$$

Also, it has the following limits for fixed $q$:

$$\lim_{P \to 0} H(P, q) = 0 ,$$
$$\lim_{P \to 1} H(P, q) = 1 , \qquad (A.4)$$
$$\lim_{P \to \infty} H(P, q) = \infty \quad (q \neq 0, 1) .$$

As a function of $q$ the function $H(P, q)$ is invariant under the transformation:

$$q \to q' \equiv \frac{1}{q} . \qquad (A.5)$$

For $P = 1$ it is constant: $H(1, q) = 1$ and for $P < 1$ ($P > 1$) it has maximum (minimum) at $q = 1$ equal to $P$. The point $P = q = 1$ is singular and the limits $\lim_{q \to 1}$ and $\lim_{P \to 1}$ do not commute. Also, the limit $\lim_{q \to 0}$ is singular — it is equal $0$ for $P \in [0, 1)$, equal $1$ for $P = 1$ and undefined for $P > 1$.

## Appendix B: A remark about $D_N$

Let us consider the function $f(\theta) = \theta$, $-\pi < \theta < \pi$. This function has the Fourier expansion:

$$\theta = \sum_{n=1}^{\infty} b_n \sin n\theta,$$

where

$$b_n = \frac{2(-1)^n}{n} .$$

Let us recall that

$$D_N(\theta) = i \sum_{n=1}^{N} \frac{2(-1)^{n+1}(N!)^2}{n(N+n)!(N-n)!} \sin n\theta.$$

The main idea now is to compare the $N$-th partial sum $S_N$ of $if(\theta)$ with the above sum. Clearly,

$$S_N(\theta) = i \sum_{n=1}^{N} \frac{2(-1)^{n+1}}{n} \sin n\theta.$$

The two sums look alike, the difference is the factor $\frac{(N!)^2}{(N-n)!(N+n)!}$.

We claim that $D_N(\theta)$ is an approximation to $i\theta$, i.e. $\lim_{N\to\infty} D_N(\theta) = i\theta$ in $(-\pi, \pi)$. This approximation is a result of a specific method of summation of the Fourier series, similar to the Fejer method of arithmetic means. Let us briefly review this subject. We refer the reader to [33] for more details. Given an infinite matrix $a = [a_{ij} : i, j = 0, 1, \ldots]$ and a sequence $\{S_n : n = 0, 1, \ldots\}$ we define a new sequence $\sigma_n, n = 0, 1, \ldots$ by

$$\sigma_N = \sum_{n=0}^{\infty} a_{Nn} S_n.$$

We require that $a$ satisfy the following conditions:

(i) $\lim_{N\to\infty} a_{Nn} = 0$.

(ii) $B_N := \sum_{n=0}^{\infty} |a_{Nn}|$ exists for every $N = 0, 1, \ldots$, and the set $\{B_N : N = 0, 1, \ldots\}$ is bounded.

(iii) $\lim_{N\to\infty} \sum_{n=0}^{\infty} a_{Nn} = 1$.

If the $\sigma_N$ have a limit $s$ then we say that the sequence of partial sums $S_N$ is $a-summable$ to the limit $s$. The most important fact for us is the following:

**Theorem B.1 [33]:** *If $a$ satisfies (i), (ii) and (iii) and if $S_N$ tends to a finite limit $s$, then $\lim_{N\to\infty} \sigma_N = s$.*

We claim that $D_N$ are precisely the linear means $\sigma_N$ for an appropriate choice of $a$. We define:

$$a_{Nn} = \begin{cases} \frac{(2n+1)(N!)^2}{(N-n)!(N+n+1)!}, & \text{if } 0 < n \leq N \text{ ;} \\ 0, & \text{otherwise.} \end{cases}$$

It is easy to check that $a$ so defined satisfy (i) and (ii). To see that (iii) is satisfied as well we observe that $a_{Nn}$ satisfy:

$$\sum_{m=n}^{N} a_{Nm} = \frac{(N!)^2}{(N-n)!(N+n)!}, \qquad 0 \leq n \leq N. \tag{B.1}$$

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In particular, for $n = 1$ we obtain:

$$\sum_{n=1}^{N} a_{Nn} = \frac{(N!)^2}{(N-1)!(N+1)!} = \frac{N}{N+1}.$$

By taking the limit $N \to \infty$ we obtain (iii). To prove our claim we need to show that $D_N = \sigma_N$. This follows from $(B.1)$. Finally, applying Theorem B.1 we conclude that $\lim_{N \to \infty} D_N(\theta) = i\theta$.

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